Mixed-state fidelity and quantum criticality at finite temperature

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(Dated: February 9, 2008)

We extend to finite temperature the fidelity approach to quantum phase transitions (QPTs). This is done by resorting to the notion of mixed-state fidelity that allows one to compare two density matrices corresponding to two different thermal states. By exploiting the same concept we also propose a finite-temperature generalization of the Loschmidt echo. Explicit analytical expressions of these quantities are given for a class of quasi-free fermionic Hamiltonians. A numerical analysis is performed as well showing that the associated QPTs show their signatures in a finite range of temperatures.

I. INTRODUCTION

Even, small and smooth changes in parameters governing the dynamics of a physical system can, in some circumstances, result in a dramatic change of physical properties of the system itself. The traditional approach to these so-called critical phenomena is based on the notions of order parameter, correlation functions, symmetry breaking, and a general formulation in the framework of the Landau-Ginzuburg picture and renormaliztion group [1]. A *phase transition* can be triggered e.g., by a change of temperature of the system or, at zero temperature, by a change of some of the coupling constants (e.g., external fields) defining the system's Hamiltonian. In the first case one says that the transition is driven by thermal fluctuations, and the transition is referred to as *classical*, whereas in the second quantum fluctuations are held responsible for the transition and this latter is referred to as a *quantum phase transition* (QPT) [2].

In the last few years a big deal of interest has grown about the possibility of studying QPTs by means of ideas and tools borrowed from the new born field of Quantum Information Science [3]. In this novel approach the key concept involved is quantum entanglement (or genuinely quantum correlations) and the idea is that quantum criticality can be suitably characterized in terms of the behavior of different entanglement measures [4]. Though the picture is still rapidly moving it is by now clear that, whereas there are no doubts that entanglement is indeed a valuable conceptual tool to analyze QPTs, one has, case by case, identify what is the entanglement measure e.g., block-entanglement or concurrence most suited to extract the relevant information.

More recently an approach to QPTs based on another quantum information notion i.e., *quantum fidelity*, has been put forward [5, 6]. The idea behind this novel approach is quite simple: the dramatic chance of the structure of the ground state occurring at the critical points can be fruitfully studied by analyzing their degree of distinguishability. Since this latter quantity is related to the overlap i.e., scalar product, between two different ground states, the fidelity approach is basically nothing but than a *metric* one; the key ingredient being provided by the state-space distance between states corresponding to two slightly different sets of coupling constants. The expectation is that at the critical points a small change of the control parameters should result in an enhanced modification of the state structure and this in turn should be detected by a greater state-space distance i.e., statistical distinguishabiliy, between the associated quantum states. In spite of its apparent naivety, this metric-based approach turns out to be able to provide an effective way to obtain, qualitative as well as quantitative, information about the zero-temperature phase diagram of a large class of non trivial quantum systems i.e., quasi-free fermionic systems [6] and matrix-product states [7]. The conceptual appealing of the fidelity approach for detecting boundaries between different phases lie in its universal geometrical as well as information-theoretic nature; in principle no apriori knowledge of the symmetry-breaking mechanism and of the associated order parameters is required.

In this paper we are going to extend the fidelity approach to *finite temperature*. This generalization can be achieved by exploiting the mixed-state fidelity introduced by Uhlmann [8] and related to the statistical distance between two density operators (Bures distance). This finite temperature extension of the fidelity approach is a nontrivial technical step necessary to analyze the signatures of QPTs at non zero temperature and, more in general, to investigate the potential usefulness of the fidelity notion in the study of classical i.e., temperature-driven phase transitions [9]. In the following we will focus on the first task. Moreover, we will provide an explicit finite-temperature extension of another concept that has been recently used in the context of QPTs and inspired the whole fidelity programme: the Loschmidt echo [10, 11].

The paper is organized as follows: In Sec. II, we analytically calculate the mixed-state fidelity of thermal states and a numerical analysis is used to demonstrate

the signatures of QPTs at finite temperature. In Sec. III, we calculate the Loschmidt echo through a similar procedure. Sec. IV contains the conclusion.

II. MIXED-STATE FIDELITY OF THERMAL STATES

Let us consider the set of (mixed) quantum states $\mathcal{S}(\mathcal{H}) := \{\rho \in \mathcal{L}(\mathcal{H}) / \rho \geq 0, \mathrm{tr}\rho = 1\}$. The mixed-state fidelity is given by [8]

$$F(\rho_0, \rho_1) := \mathrm{tr}\sqrt{\rho_1^{\frac{1}{2}} \rho_0 \rho_1^{\frac{1}{2}}}. \quad (1)$$

This quantity measures the degree of distinguishability between the two quantum states ρ_0 and ρ_1. The fidelity is related to the statistical Bures distance: $D(\rho_0, \rho_1) = \sqrt{2(1-F)}$. We will use Eq. (1) to compare two different thermal states

$$\begin{aligned} \rho_\alpha &= Z_\alpha^{-1} \exp(-\beta_\alpha H_\alpha), \\ Z_\alpha &: = \mathrm{tr} \exp(-\beta_\alpha H_\alpha), (\alpha = 0, 1). \end{aligned} \quad (2)$$

We define

$$\mathcal{F}_{H_0, H_1}(\beta_0, \beta_1) := F\left(Z_0^{-1} e^{-\beta_0 H_0}, Z_1^{-1} e^{-\beta_1 H_1}\right). \quad (3)$$

In particular one can consider the cases

- (i) $H_\alpha = H(\lambda_\alpha), \lambda_1 = \lambda_0 + \delta\lambda; \beta_0 = \beta_1 = \beta$.

- (ii) $H_\alpha = H(\beta_\alpha), \beta_1 = \beta_0 + \delta\beta$.

The first case (i) is useful to study the finite-temperature signatures of a QPT occurring at some points, say λ_c, in the parameter space. The second case (ii) is considered for studying temperature driven phase transitions. Here the β dependence of the Hamiltonian can be the result of the presence of e.g., a chemical potential term (grand canonical ensemble) or of self-consistently determined coupling e.g., a mean-field BCS pairing term. In this paper we will focus on case (i), while the use of mixed-state fidelity for analyzing temperature driven PTs will be addressed in a forthcoming work.

A. Commuting Hamiltonians

Let us start by considering the simple case where the two Hamiltonians H_0 and H_1 commute; then

$$\rho_1^{\frac{1}{2}} \rho_0 \rho_1^{\frac{1}{2}} = \rho_1 \rho_0 = (Z_0 Z_1)^{-1} \exp(-\beta_0 H_0 + \beta_1 H_1). \quad (4)$$

Therefore by using the definition (1)

$$\begin{aligned} &F(\rho_0, \rho_1) \\ &= (Z_0 Z_1)^{-1/2} \mathrm{tr} \exp\left[-(\beta_0 H_0 + \beta_1 H_1)/2\right] \\ &= (Z_0 Z_1)^{-1/2} \sum_n \exp(-(\beta_0 E_n^0 + \beta_1 E_n^1)/2), \quad (5) \end{aligned}$$
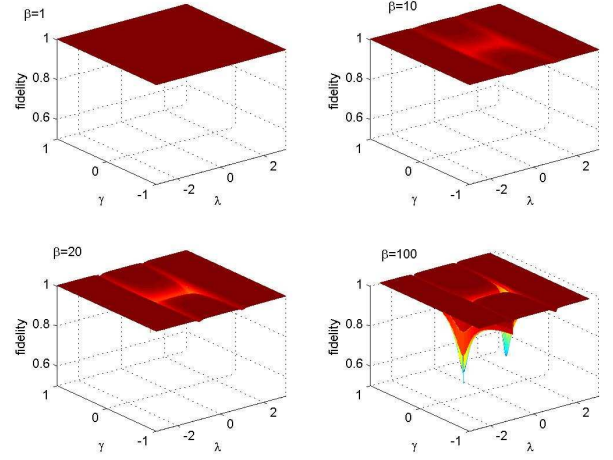

FIG. 1: (Color online) Mixed-state fidelity of finite-temperature thermal state of the XY model. The fidelity is a function of λ and γ. Here, we choose the spin number $N = 200$ and the parameter perturbation $\delta\lambda = \delta\gamma = 10^{-2}$. The temperatures of system in the above four figures are chosen to be $\beta = 1, \beta = 10, \beta = 20,$ and $\beta = 100$, respectively. At low temperatures, e.g., $\beta = 100$, the mixed-state fidelity clearly shows the signature of QPT which occurs at absolute zero temperature. When the temperature increases, the decay of fidelity becomes less sharp and finally the signature of QPT disappears due to the thermal excitation.
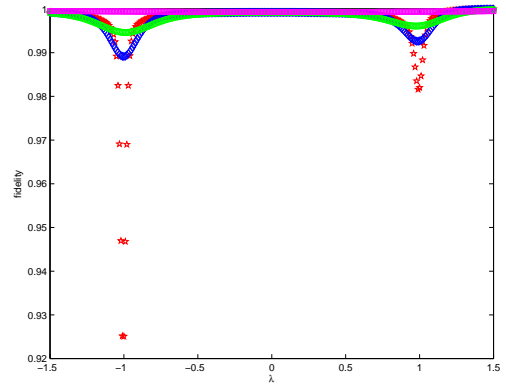

FIG. 2: (Color online) A cross section of Fig. 1 with $\gamma = 1$, i.e., mixed state fidelity of finite-temperature thermal state of transverse Ising model. Here, the same as that in Fig. 1, the spin number is chosen to be $N = 200$ and the parameter perturbation $\delta\lambda = \delta\gamma = 10^{-2}$. Four curves represent four different temperatures: $\beta = 1, \beta = 10, \beta = 20,$ and $\beta = 100$ respectively. The decay of fidelity, though becomes less sharp with the increase of the temperature, well indicates the critical point of the transverse Ising model.

where $H_\alpha|\Psi_n\rangle = E_n^\alpha|\Psi_n\rangle (\alpha = 0, 1)$. In particular if moreover $H_0 = H_1$ one immediately finds that fidelity of thermal states can be expressed entirely in terms of partition functions

$$\mathcal{F}(\beta_0, \beta_1) = \frac{Z(\frac{\beta_0 + \beta_1}{2})}{\sqrt{Z(\beta_0) Z(\beta_1)}}. \tag{6}$$

We note in passing that this relation seems to suggest the possibility of making a direct connection between the metric/statistical notion of fidelity and purely thermodynamical quantities as well as the viability of the fidelity approach even for classical systems [9]. We would like also to observe that Eq (6) also gives the (pure-state) fidelity between the pure quantum states that one associates to the thermal states ρ_0 and ρ_1 through the kind of classical-quantum correspondence discussed in [12] [see Eq (1) there].

To further exemplify this commuting case let us consider diagonal fermionic Hamiltonians $H_\alpha = \sum_k \epsilon_k^\alpha c_k^\dagger c_k$. One has

$$\begin{aligned} \rho_\alpha(\beta) &= Z_\alpha^{-1} \prod_k e^{-\beta_\alpha \epsilon_k^\alpha c_k^\dagger c_k} \\ &= \prod_k (1 + e^{-\beta_\alpha \epsilon_k^\alpha})^{-1} \left[1 + (e^{-\beta_\alpha \epsilon_k^\alpha} - 1) c_k^\dagger c_k\right]. \end{aligned}$$

From this one finds

$$\mathcal{F}_{H_0, H_1}(\beta_0, \beta_1) = \prod_k \frac{1 + e^{-(\beta_0 \epsilon_k^0 + \beta_1 \epsilon_k^1)/2}}{\sqrt{(1 + e^{-\beta \epsilon_k^0})(1 + e^{-\beta \epsilon_k^0})}}. \tag{7}$$

In the zero-temperature limit $\beta \to \infty$, from the above equation, it is easy to check that $\forall k, \epsilon_k^0 \epsilon_k^1 \geq 0 \Rightarrow \mathcal{F}_{H_0, H_1}(\infty, \infty) = 1$, wheras if $\exists k, \epsilon_k^0 \epsilon_k^1 < 0 \Rightarrow \mathcal{F}_{H_0, H_1}(\infty, \infty) = 0$. This situation is the one that encounters in the XY-model analysis of [5] in the critical line with anisotropic parameter $\gamma = 0$. There indeed when the magnetic field λ (which plays the role of a chemical potential in the fermionic picture) is changed in the range $[-1, 1]$ one has exactly that one of the single particle eigenvalues changes sign and this results in a vanishing fidelity [5].

B. A more general case

Now we move to consider a more general case directly relevant to the XY and mean-field BCS-like models. The Hamiltonian is given by

$$H^\alpha = \sum_k H_k^\alpha = \sum_k \epsilon_k^\alpha(n_k + n_{-k}) + \Delta_k^\alpha(-ic_k^\dagger c_{-k}^\dagger + \text{h.c.}), \tag{8}$$

where $n_k := c_k^\dagger c_k$ and the c_k's are fermionic operators i.e., $\{c_k, c_{k'}^\dagger\} = \delta_{k,k'}$. The Hilbert space factorizes $\mathcal{H} = \otimes_k \mathcal{H}_k$. One has $\mathcal{H}_k \otimes \mathcal{H}_{-k} = \text{span}\{|00\rangle_{k,-k}, |11\rangle_{k,-k}, |01\rangle_{k,-k}, |10\rangle_{k,-k}\}$. The first

(last) two vectors span the even (odd) parity sector. The Hamiltonian (8) has a trivial action over the odd sector i.e., $H_k^\alpha|_{odd} = \epsilon_k^\alpha \mathbb{1}_{k,-k}$. Therefore, neglecting irrelevant constants one can write

$$H_k^\alpha = 2\epsilon_k^\alpha J_k^z + 2\Delta_k^\alpha J_k^y, \tag{9}$$

where $J_k^z := 1/2(n_k + n_{-k} - 1)$, $J_k^y := 1/2\left(-ic_k^\dagger c_{-k}^\dagger + \text{h.c.}\right)$. For every k, the operators $J_k^x := 1/2(c_k^\dagger c_{-k}^\dagger + \text{h.c.})$, J_k^y, J_k^z span a $su(2)$ Lie-algebra such that the even (odd) sector of $\mathcal{H}_k \otimes \mathcal{H}_{-k}$ is the $J = 1/2$ $(J = 0)$ irreducible representation. Therefore, with obvious notation one can write

$$\begin{aligned} H_k^\alpha &= (\epsilon_k^\alpha \sigma^z + \Delta_k^\alpha \sigma_k^y) \oplus 0_2 = \Lambda_k^\alpha J_k^\alpha \oplus 0_2 \\ &= \left(e^{i\frac{\theta_k^\alpha}{2}\sigma_{kx}} \Lambda_k^\alpha \sigma_{kz} e^{-i\frac{\theta_k^\alpha}{2}\sigma_{kx}}\right) \oplus 0_2. \end{aligned} \tag{10}$$

where

$$\begin{aligned} \Lambda_k^\alpha &:= \sqrt{(\epsilon_k^\alpha)^2 + (\Delta_k^\alpha)^2}, \\ J_k^\alpha &:= \cos\theta_k^\alpha \sigma^z + \sin\theta_k^\alpha \sigma_k^y, \\ \theta_k^\alpha &:= \tan^{-1}(\Delta_k^\alpha/\epsilon_k^\alpha). \end{aligned}$$

Moreover,

$$\begin{aligned} \exp(-\beta_\alpha H_k^\alpha) &= \varrho_k^\alpha(\beta_\alpha) \oplus \mathbb{1}_{k,-k}, \\ \rho_\alpha &= \prod_k (Z_k^\alpha)^{-1} \varrho_k^\alpha(\beta_\alpha) \oplus \mathbb{1}_{k,-k} \end{aligned} \tag{11}$$

where

$$\begin{aligned} \varrho_k^\alpha(\beta) &:= \exp(-\beta \Lambda_k^\alpha J_k^\alpha) \\ &= \cosh(\beta \Lambda_k^\alpha) - J_k^\alpha \sinh(\beta \Lambda_k^\alpha) \end{aligned} \tag{12}$$

is a 2×2 operator in the even sector, and

$$Z_k^\alpha = 2 + 2\cosh(\beta \Lambda_k^\alpha). \tag{13}$$

The fidelity for the two thermal states is then given by

$$\begin{aligned} &\mathcal{F}_{H_0, H_1}(\beta_0, \beta_1) \\ &= \prod_k \frac{2 + \text{tr}\sqrt{\varrho_k^1(\beta_1)^{\frac{1}{2}} \varrho_k^0(\beta_0) \varrho_k^1(\beta_1)^{\frac{1}{2}}}}{\sqrt{Z_k^0 Z_k^1}}. \end{aligned} \tag{14}$$

So, apart for the trivial terms in the odd sector in order to compute the fidelity, one has to consider the products $\varrho_k^1(\beta_1/2)\varrho_k^0(\beta_0)\varrho_k^1(\beta_1/2)$. As this is a product of 2×2 matrices, one has

$$\begin{aligned} &\text{tr}\sqrt{\varrho_k^1(\beta_1)^{\frac{1}{2}} \varrho_k^0(\beta_0) \varrho_k^1(\beta_1)^{\frac{1}{2}}} \\ &= \sqrt{\text{Tr}\left[\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)\right] + 2\det(\varrho_k^0(\beta_0)\varrho_k^1(\beta_1))} \end{aligned}$$

Note that here $\det(\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)) = 1$, then substituting the above equation to Eq.(14) leads to a simple expression of the fidelity

$$\begin{aligned} &\mathcal{F}_{H_0, H_1}(\beta_0, \beta_1) \\ &= \prod_k \frac{2 + \sqrt{\text{Tr}\left[\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)\right] + 2}}{\sqrt{Z_k^0 Z_k^1}}. \end{aligned} \tag{15}$$

Now, we are left to compute the trace of $\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)$.

The matrix product $\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)$ can be written as

$$\text{Tr}\left[\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)\right]$$
$$= \text{Tr}\left(e^{-\beta_0\Lambda_k^0\sigma_{kz}}e^{i\alpha_k\sigma_{kx}}e^{-\beta_1\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}\right)$$
$$= \text{Tr}\left(\left[\cosh(\beta_0\Lambda_k^0) - \sinh(\beta_0\Lambda_k^0)\sigma_{kz}\right]\right.$$
$$\left.\times e^{i\alpha_k\sigma_{kx}}e^{-\beta_1\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}\right)$$
$$= 2\cosh(\beta_0\Lambda_k^0)\cosh(\beta_1\Lambda_k^1) - \sinh(\beta_0\Lambda_k^0)$$
$$\times\text{Tr}\left(e^{-i\alpha_k\sigma_{kx}}\sigma_{kz}e^{-\beta_1\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}\right), \qquad (16)$$

where $\alpha_k = \frac{\theta_k^1 - \theta_k^0}{2}$.

The following trace can be evaluated as

$$\text{Tr}\left(e^{-i\alpha_k\sigma_{kx}}\sigma_{kz}e^{-\beta_1\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}\right)$$
$$= \text{Tr}\left(e^{-i2\alpha_k\sigma_{kx}}\left[\sigma_{kz}\cosh(\beta_1\Lambda_k^1) - \sinh(\beta_1\Lambda_k^1)\right]\right)$$
$$= \cosh(\beta_1\Lambda_k^1)\text{Tr}\left(e^{-i2\alpha_k\sigma_{kx}}\sigma_{kz}\right) - 2\sinh(\beta_1\Lambda_k^1)\cos(2\alpha_k)$$
$$= -2\sinh(\beta_1\Lambda_k^1)\cos(2\alpha_k) \qquad (17)$$

Substituting Eq.(17) to (16) leads to

$$\text{Tr}\left[\varrho_k^0(\beta_0)\varrho_k^1(\beta_1)\right]$$
$$= 2[\cosh(\beta_0\Lambda_k^0)\cosh(\beta_1\Lambda_k^1)$$
$$+ \sinh(\beta_0\Lambda_k^0)\sinh(\beta_1\Lambda_k^1)\cos(\theta_k^0 - \theta_k^1)].$$

Bringing all the terms together one eventually finds

$$\mathcal{F}_{H_0,H_1}(\beta_0,\beta_1)$$
$$= \prod_k\left\{\left[1 + \cosh(\beta_0\Lambda_k^0)\right]\left[1 + \cosh(\beta_1\Lambda_k^1)\right]\right\}^{-\frac{1}{2}}$$
$$\times(1 + \frac{1}{\sqrt{2}}[1 + \cosh(\beta_0\Lambda_k^0)\cosh(\beta_1\Lambda_k^1)$$
$$+ \sinh(\beta_1\Lambda_k^0)\sinh(\beta_1\Lambda_k^1)\cos(\theta_k^0 - \theta_k^1)]^{\frac{1}{2}}) \qquad (18)$$

It is easy to check that

$$\mathcal{F}_{H_0,H_1}(\beta,\beta) \overset{\beta\to\infty}{\to} \prod_k\sqrt{\frac{1 + \cos(\theta_k^0 - \theta_k^1)}{2}}$$
$$= \prod_k\left|\cos(\frac{\theta_k^0 - \theta_k^1}{2})\right| \qquad (19)$$

i.e., one recovers the zero-temperature result [5].

C. Numerical analysis

We use XY model as an example to demonstrate our main idea. Here, two Hamiltonians are $H_0 = H(\gamma,\lambda)$ and $H_1 = H(\gamma + \delta\gamma, \lambda + \delta\lambda)$ where

$$H(\gamma,\lambda) = \sum_i\left[\frac{1+\gamma}{2}\sigma_i^x\sigma_{i+1}^x + \frac{1-\gamma}{2}\sigma_i^y\sigma_{i+1}^y + \lambda\sigma_i^z\right],$$
$$(20)$$

where γ defines the anisotropy and λ represents external magnetic field along the z axis. Obviously, when $\gamma = 1$, the XY Hamiltonian (20) reduce to the transverse Ising Hamiltonian. $\delta\gamma$ and $\delta\lambda$ represent small perturbation to the Hamiltonian. σ_i^α, $\alpha \in \{x,y,z\}$ are usual Pauli operators in the i-th lattice point. It is well known that this model, by means of a Jordan-Wigner transformation, can be mapped onto a quasi-free fermionic Hamiltonian of the type (8) [i.e., $\epsilon_k = \cos\frac{2k\pi}{N} - \lambda$, $\Delta_k = \gamma\sin\frac{2k\pi}{N}$]. Through a straightforward calculation, it can be obtained that $\Lambda_k^0 = \Lambda_k(\gamma,\lambda)$ and $\Lambda_k^1 = \Lambda_k(\gamma + \delta\gamma, \lambda + \delta\lambda)$ where

$$\Lambda_k^0 = \sqrt{\left[\cos\frac{2k\pi}{N} - \lambda\right]^2 + \gamma^2\sin^2\frac{2k\pi}{N}}, \qquad (21)$$

and $\theta_k^\alpha = \cos^{-1}[(\cos\frac{2k\pi}{N} - \lambda_\alpha)/\Lambda_k^\alpha]$, $(\alpha = 0,1, \lambda_0 = \lambda, \lambda_1 = \lambda + \delta\lambda)$. We plot the mixed-state fidelity according to the analytical expression obtained above (18). We choose the number of spins to be 200, and the perturbation to be 10^{-2}. In Fig. 1, we consider four different temperatures; $\beta = 1$, $\beta = 10$, $\beta = 20$, and $\beta = 100$, respectively. At low temperature, e.g., $\beta = 100$, the sharp decay of fidelity in critical region clearly displays the QPT, which happens at zero temperature. What is more, the pattern of fidelity in low temperature is very similar to the ground-state fidelity [5] of the XY model. This similarity is natural because, as we mentioned above, the mixed-state fidelity approaches ground-state fidelity when the temperature decreases to zero. When the temperature increases higher, e.g., $\beta = 10$ or $\beta = 20$, the decay of fidelity, though less sharp due to the thermal excitation, still early shows the signature of QPT. However, when the temperature becomes large enough, e.g., $\beta = 1$, the dramatic decay of ground-state fidelity at critical point is totally washed out by the thermal excitation and the signature of QPT at critical point eventually disappears. In Fig. 2, we plot the mixed-state fidelity of thermal state of the transverse Ising model. This is actually a cross section of Fig. 1 at $\gamma = 1$. The decay of fidelity clearly indicate the critical point of transverse Ising system.

It is important to stress that these numerical findings, besides illustrating the possibility of detecting and studying the finite-temperature signatures of QPTs, show that the ground-state fidelity approach to criticality is endowed with some robustness against "perturbations" of the ground state. In this case, in fact we have seen that mixing the ground state with excited eigenstates does not destroy the peculiar behavior of fidelity in the neighborhood of the QPTs i.e.,the fidelity drop.

III. LOSCHMIDT ECHO

In Refs. [10] and [11], the concept of Loschmidt echo has been used to investigate quantum criticality. The resulting picture is that the asymptotic value of the
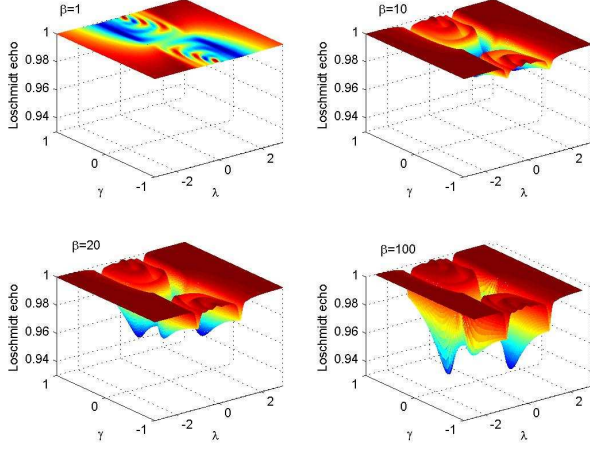
FIG. 3: (Color online) Mixed-state Loschmidt echo finite-temperature thermal state of the XY model at an instant $t = 10$. Here, we choose the spin number $N = 200$ and the parameter perturbation $\delta\lambda = \delta\gamma = 10^{-2}$. The temperatures of system in the above four figures are chosen to be $\beta = 1, \beta = 10, \beta = 20$, and $\beta = 100$, respectively. Similar to the mixed-state fidelity approach, the critical region is well indicated by Loschmidt echo at an instant when the system is at a low temperature. However, the signature of QPT disappears when the temperature increases to very high value.
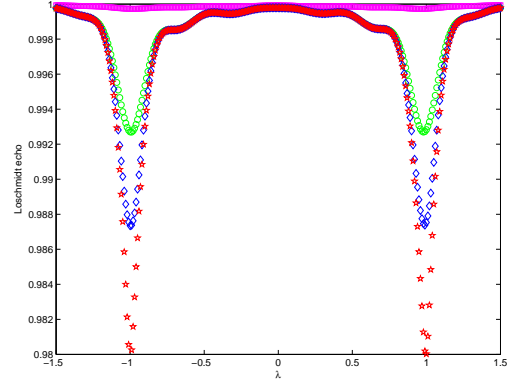
FIG. 4: (Color online) A cross section of Fig. 3 with $\gamma = 1$, i.e., mixed-state Loschmidt echo (at an instant) of finite-temperature thermal state of transverse Ising model. Here, the same as that in Fig. 3, the spin number is chosen to be $N = 200$ and the parameter perturbation $\delta\lambda = \delta\gamma = 10^{-2}$. Four curves represent four different temperatures: $\beta = 1, \beta = 10, \beta = 20$, and $\beta = 100$, respectively. The critical point is well indicated by Loschmidt echo when the temperature is not too high.

Loschmidt echo (for infinitely long times) is directly related to the closeness of the system to the critical points i.e., the closer the systems to the QPT the smaller the asymptotic value of the Loschmidt echo. On the other hand, even the short time behavior brings about information about the QPTs. Indeed, for short times the decay of the Loschmidt echo appears to be gaussian $\sim \exp(-\alpha t^2)$, where the rate α has a diverging derivative (as a function of e.g., magnetic field) at the critical point [11].

Now we show how to generalize the notion of Loschmidt echo in a natural way to the thermal state case. This natural extension to the realm of mixed-state can be obtained by using Eq. (1),

$$L_{\rho_{in}, H_0, H_1}(t) := F(\rho_{in}, U_1(t)^\dagger U_0(t)\rho_{in}U_0^\dagger(t)U_1(t)),$$
$$U_\alpha := \exp(-iH_\alpha t) \quad (\alpha = 0, 1). \quad (22)$$

In particular, one can chose $\rho_{in} = \exp(-\beta H_0)$, then Eq. (22) simplifies and one can define

$$\mathcal{L}_{H_0, H_1}(\beta, t) = F\left[Z_0^{-1}e^{-\beta H_0}, Z_0^{-1}U_1^\dagger(t)e^{-\beta H_0}U_1(t)\right]$$
$$= Z_0^{-1}F\left[e^{-\beta H_0}, U_1^\dagger(t)e^{-\beta H_0}U_1(t)\right]$$
$$= \mathcal{F}_{H_0, U_1^\dagger(t)H_0 U_1(t)}(\beta, \beta). \quad (23)$$

Then, from the above equation and Eq. (15), one finds

$$\mathcal{L}_{H_0, H_1}(\beta, t) = \prod_k \left(Z_k^0\right)^{-1}\left(2 + \sqrt{\text{Tr}\left[\varrho_k^0(\beta)\varrho_k^1(\beta)\right] + 2}\right)$$
$$(24)$$

with

$$\varrho_k^0(\beta) = e^{i\frac{\theta_k^0}{2}\sigma_{kx}}e^{-\beta\Lambda_k^0\sigma_{kz}}e^{-i\frac{\theta_k^0}{2}\sigma_{kx}},$$
$$\varrho_k^1(\beta) = U_1^\dagger(t)e^{i\frac{\theta_k^0}{2}\sigma_{kx}}e^{-\beta\Lambda_k^0\sigma_{kz}}e^{-i\frac{\theta_k^0}{2}\sigma_{kx}}U_1(t). \quad (25)$$

Notice now that the unitary operator $U_1(t)$ can be written as $U_1(t) = e^{i\frac{\theta_k^1}{2}\sigma_{kx}}e^{-i\Lambda_k^1 t\sigma_{kz}}e^{-i\frac{\theta_k^1}{2}\sigma_{kx}}$. Then,

$$\text{Tr}\left[\varrho_k^0(\beta)\varrho_k^1(\beta)\right]$$
$$= \text{Tr}(e^{i\frac{\theta_k^0}{2}\sigma_{kx}}e^{-\beta\Lambda_k^0\sigma_{kz}}e^{-i\frac{\theta_k^0}{2}\sigma_{kx}}e^{i\frac{\theta_k^1}{2}\sigma_{kx}}e^{it\Lambda_k^1\sigma_{kz}}e^{-i\frac{\theta_k^1}{2}\sigma_{kx}}$$
$$\times e^{i\frac{\theta_k^0}{2}\sigma_{kx}}e^{-\beta\Lambda_k^0\sigma_{kz}}e^{-i\frac{\theta_k^0}{2}\sigma_{kx}}e^{i\frac{\theta_k^1}{2}\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}}e^{-i\frac{\theta_k^1}{2}\sigma_{kx}})$$
$$= \text{Tr}(e^{-\beta\Lambda_k^0\sigma_{kz}}e^{i\alpha_k\sigma_{kx}}e^{it\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}$$
$$e^{-\beta\Lambda_k^0\sigma_{kz}}e^{i\alpha_k\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}})$$
$$= \text{Tr}(e^{-\beta\Lambda_k^0\sigma_{kz}}e^{-\beta\Lambda_k^0 V^\dagger\sigma_{kz}V}), \quad (26)$$

where $V = e^{i\alpha_k\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}$. Using the formula $e^x = \cosh x - \sinh x$, one have

$$\text{Tr}\left[\varrho_k^0(\beta)\varrho_k^1(\beta)\right]$$
$$= 2\cosh^2(\beta\Lambda_k^0) + \sinh^2(\beta\Lambda_k^0)\text{Tr}(\sigma_{kz}V^\dagger\sigma_{kz}V). \quad (27)$$

The following trace is evaluated as

$$\text{Tr}(\sigma_{kz}V^\dagger\sigma_{kz}V)$$
$$= \text{Tr}(\sigma_{kz}e^{i\alpha_k\sigma_{kx}}e^{it\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}}$$
$$\times\sigma_{kz}e^{i\alpha_k\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}}e^{-i\alpha_k\sigma_{kx}})$$
$$= \text{Tr}(\sigma_{kz}e^{i\alpha_k\sigma_{kx}}e^{it\Lambda_k^1\sigma_{kz}}e^{-i2\alpha_k\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}}e^{i\alpha_k\sigma_{kx}}\sigma_{kz})$$
$$= \text{Tr}(e^{i2\alpha_k\sigma_{kx}}e^{it\Lambda_k^1\sigma_{kz}}e^{-i2\alpha_k\sigma_{kx}}e^{-it\Lambda_k^1\sigma_{kz}})$$
$$= \text{Tr}(\left[\cos(t\Lambda_k^1)+i\sin(\Lambda_k^1 t)e^{i2\alpha_k\sigma_{kx}}\sigma_{kz}e^{-i2\alpha_k\sigma_{kx}}\right]$$
$$\times\left[\cos(t\Lambda_k^1)-i\sin(t\Lambda_k^1)\sigma_{kz}\right])$$
$$= 2\cos^2(t\Lambda_k^1)+\sin^2(t\Lambda_k^1)\text{Tr}(\sigma_{kz}e^{i2\alpha_k\sigma_{kx}}\sigma_{kz}e^{-i2\alpha_k\sigma_{kx}})$$
$$= 2\cos^2(t\Lambda_k^1)+2\sin^2(t\Lambda_k^1)\cos(4\alpha_k) \tag{28}$$

Substituting the above equation to Eq.(27) leads to

$$\text{Tr}\left[\varrho_k^0(\beta)\varrho_k^1(\beta)\right]$$
$$= 2\cosh^2(\beta\Lambda_k^0)+2\sinh^2(\beta\Lambda_k^0)$$
$$\times\left[\cos^2(t\Lambda_k^1)+\sin^2(t\Lambda_k^1)\cos(4\alpha_k)\right]$$
$$= 2\left[1-\sin^2(2\alpha_k)\sin^2(\Lambda_k^1 t)\right]\cosh(2\beta\Lambda_k^0)$$
$$+2\sin^2(2\alpha_k)\sin^2(\Lambda_k^1 t). \tag{29}$$

Bringing all the terms together, we give an explicit expression for the Loschmidt echo for the class of Hamiltonians (8)

$$\mathcal{L}_{H_0,H_1}(\beta,t) \tag{30}$$
$$= \prod_k\left[1+\cosh(\beta\Lambda_k^0)\right]^{-1}$$
$$\times\{1+\frac{1}{\sqrt{2}}\{\left[1-\sin^2(\theta_k^0-\theta_k^1)\sin^2(\Lambda_k^1 t)\right]$$
$$\times\cosh(2\beta\Lambda_k^0)+\sin^2(\theta_k^0-\theta_k^1)\sin^2(\Lambda_k^1 t)+1\}^{1/2}\}$$

It is immediate to check that in the zero temperature limit one recovers the result obtained in [10],

$$\mathcal{L}_{H_0,H_1}(\beta,t)\overset{\beta\to\infty}{\Rightarrow}\prod_k\sqrt{(1-\sin^2(\theta_k^0-\theta_k^1)\sin^2(\Lambda_k^1 t))}.$$

A. Numerical analysis

Similarly to Sec. II, we now study mixed-state Loschmidt echo given by Eq. (30). In Fig. 3, we plot the Loschmidt echo at an instant $t=10$. The parameters are the same as that in Fig. 1 and Fig. 2. Similar to the ground-state Loschmidt echo in Ref. [10], the decay of mixed-state Loschmidet echo of a thermal state at a finite temperature well indicates the critical point. With

the increase of the temperature, the decay of the mixed-state Loschmidt echo at critical point becomes less sharp until finally disappears. Fig. 4 is a cross section of Fig. 3 at $\gamma=1$, i.e., a mixed-state Loschmidt echo of transverse Ising model. Similarly to the mixed-state Fidelity of transverse Ising model in Fig. 2, the critical point is clearly indicated by the Loschmidt echo. With temperature increase, the decay of Loschmidt echo at critical point becomes less evident, and finally disappears for sufficiently high temperature.

IV. CONCLUSIONS

In this paper we have shown how to extend to finite temperature the fidelity approach to quantum phase transitions advocated in References [5] and [6]. This generalization relies on the notion of mixed state fidelity applied to (Gibbs) thermal states. Mixed-state fidelity is strictly related to the Bures metric measuring the statistical distance between two density operators, therefore this approach has a geometrical as well as an operational meaning and two of them are deeply intertwined. We provided an explicit analytical expression for both the fidelity and Loschmidt echo for an important class of quasi-free fermionic Hamiltonians including e.g., the XY model. A numerical analysis of these quantities has been performed; it clearly shows how the influence of the zero-temperature critical points extend over a finite range of temperatures. Besides representing a non-trivial generalization of the former zero-temperature results, the findings reported in this paper suggest directions for further investigations. The most prominent being the possibility of using (mixed) state-space metrical quantities to study temperature driven phase transitions both in the quantum and in the classical case [9]. The fact that simple geometrical notions seme to provide a unified frame for studying all these different kinds of critical phenomena is, we believe, conceptually quite appealing.

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